



Structure and mechanical properties of a light-weight AlNbTiV high entropy alloy



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ABSTRACT

The crystal structure, microstructure, density, microhardness and mechanical properties of new AlNbTiV high entropy alloy were examined. The alloy had coarse-grained single bcc phase structure with density of 5.59 g cm⁻³ and hardness of 4315–4394 MPa. The compressive yield strength of the alloy gradually decreased from 1020 MPa at room temperature to 685 MPa at 800 °C, and then dropped to 158 MPa at 1000 °C. Specific yield strength of the alloy was found to be comparable with strength of multiphase refractory high entropy alloys. Effect of chemical composition on mechanical properties and potential ways to optimize composition are discussed.

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1. Introduction

The so-called high entropy alloys (HEAs) is a new emerging class of metallic alloys which are frequently considered as potential structural materials for high-temperature applications [1]. In order to fully utilize potential of HEAs as high-temperature material, Senkov et al. has introduced refractory HEAs [2]. Several refractory HEAs compositions have demonstrated remarkable compressive strength at elevated temperatures [3,4] but had large density of more than $\approx 10 \text{ g cm}^{-3}$. The alloys of Cr–Nb–Ti–V–Zr system with lower density of $\approx 6.5 \text{ g cm}^{-3}$ and attractive mechanical properties were introduced in order to provide lighter materials [5,6]. Addition of Al as an alloying element has the potential to further decrease density of alloys [7,8]; however Al tends to form intermetallic compounds with constitutive elements of the Cr–Nb–Ti–V–Zr system. On the other hand, Al has similar atomic radii (143 pm) to those of Ti, Nb and V, which is expected to simulate formation of solid solutions in HEAs [9]. Formation of either solutions or intermetallics will significantly affect mechanical properties of alloys. In current work we report microstructure, density, and mechanical properties of novel, presumably light-weight AlNbTiV alloy.

2. Experimental procedures

The alloy with nominal composition of AlNbTiV was produced by arc melting of the high-purity ($\geq 99.9 \text{ (at)\%}$) elements in a argon

atmosphere inside a water-cooled copper cavity. Produced ingot with dimensions of $\approx 6 \times 15 \times 60 \text{ mm}^3$ was re-melted 5 times. The exact chemical composition of the alloy was 26.6 (at)%Al–23.8%Nb–25.1%Ti–24.5%V. After casting the alloy was homogenized at 1200 °C for 24 h in vacuumed (10^{-2} Torr) quartz tubes filled with titanium chips to prevent oxidation and cooled down on air.

Phase composition and microstructure of the alloy were studied using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The XRD analysis was performed using RIGAKU diffractometer and Cu K α radiation. Samples for SEM observations were prepared by mechanical polishing. SEM investigations were performed utilizing Quanta 200 3D microscope equipped with energy-dispersive (EDS) detector used for chemical composition measurements. Density of the alloy was measured via hydrostatic weighting. Vickers microhardness was measured using a 250 g load applied for 15 s. 20 measurements were made in each condition.

Compressive tests were performed on rectangular specimens with dimensions of $7 \times 5 \times 5 \text{ mm}^3$ using the Instron 5882 machine equipped with radial furnace. The initial strain rate was 10^{-3} s^{-1} and the temperature was of 22 °C, 600 °C, 800 °C and 1000 °C. For high temperature testing, the samples were placed in preheated furnace and held for 10 min before testing. Obvious oxidation was observed only after testing at 1000 °C. The testing was performed until the fracture of the specimen or reaching height reduction of 50%.

3. Results and discussion

The XRD patterns of the AlNbTiV alloy in as-cast and homogenized conditions are shown in Fig. 1a. The patterns show presence of only one phase with bcc lattice in both conditions with lattice

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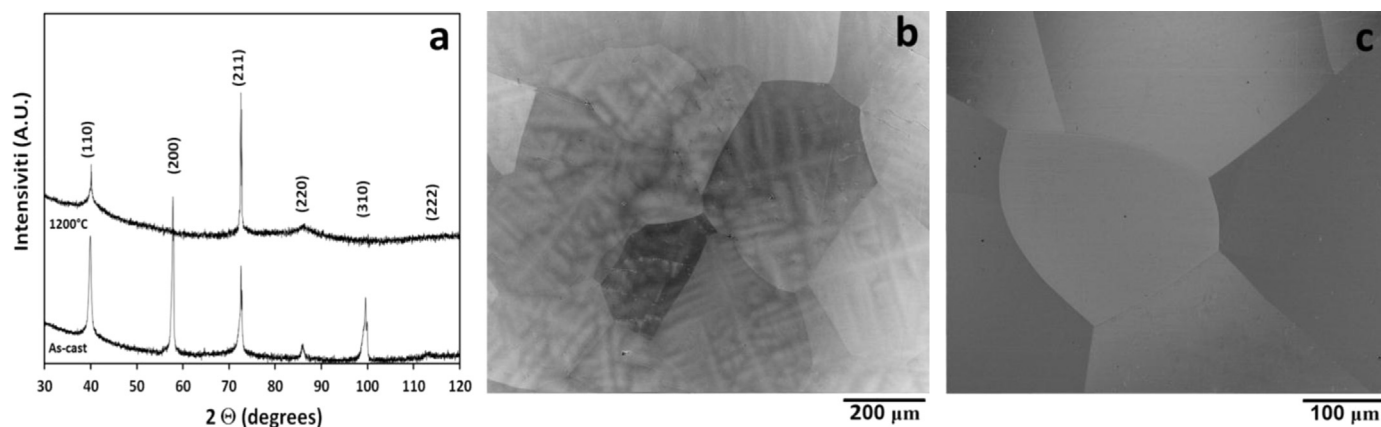


Fig. 1. Structure of the AlNbTiV alloy in as-cast and homogenized conditions: (a) XRD pattern; (b and c) SEM-BSE images: (b) as-cast condition; (c) homogenized condition.

parameter of 318 ± 3 pm. SEM image of the as-cast AlNbTiV alloy (Fig. 1b) demonstrates large grains with size of several hundred microns with dendritic structure inside. Dendrite areas (appear light on SEM image) are enriched with Nb (24.8%) and depleted of Al (26.3 (at%)) and Ti (24.3%), and interdendrite areas (dark) are enriched with Al (27.6%) and Ti (26%) and depleted of Nb (21.9%). Predominant segregation of refractory elements (i.e. Nb) in dendrite areas and lower melting temperature elements (mainly Al) in interdendrites is anticipated [10]. Complete elimination of dendritic segregations is observed after homogenization. Chemical composition of coarse grains with average size of about 300–400 μm corresponds to nominal composition of the alloy. No porosity is observed.

Formation of bcc solid solution phase instead of intermetallics in the Al-containing AlNbTiV alloy is correctly predicted by parameters $\Delta\delta = 3.14\%$ and $\Omega = 1.38$ ($\Delta\delta < 6.6\%$ and $\Omega > 1.1$ are required for solid solution formation [9]) and $\text{VEC} = 4.25$ ($\text{VEC} < 6.87$ is required for BCC structure [11]). It should be mentioned that $\Delta\delta$ and Ω parameters were successfully used to predict solid solutions formations in HEAs with somewhat similar compositions [7].

The measured density of the AlNbTiV alloy was found to be of 5.59 g cm^{-3} and is slightly higher than the density predicted by the rule of mixtures, 5.39 g cm^{-3} . Somewhat higher experimentally measured density values in refractory were already reported [7]. It should be noted that the studied AlNbTiV alloy has the lowest density among reported refractory HEAs compositions [2–8,10,12–15]. No noticeable effect of annealing on microhardness was revealed; hardness was found to be of $4315 \pm 98 \text{ MPa}$ and $4394 \pm 118 \text{ MPa}$ in as-solidified and annealed conditions respectively.

The compression stress–strain curves of the homogenized AlNbTiV alloy at different temperatures are shown in Fig. 2. The resulting mechanical properties, yield strength ($\sigma_{0.2}$), peak stress (σ_u) and fracture strain, ϵ , are summarized in Table 1. At room temperature the alloy has demonstrated high yield stress of 1020 MPa, but brittle fracture occurs shortly after yielding at strain of 5% at peak stress of 1318 MPa. Increase of testing temperature to 600 °C results in decrease of yield strength to 810 MPa. Pronounced work hardening stage is observed, and specimen fails when strain reaches 12% at stress of 1050 MPa. Further increase of testing temperature to 800 °C results in continuous decrease of yield strength to 685 MPa and increase of ductility of alloy—height reduction of 50% is reached without fracture. Pronounced steady-state flow stage is observed on the stress–strain curve. The AlNbTiV alloy behaves similarly during mechanical testing at 1000 °C, however, substantial decrease of yield strength to 158 MPa is observed.

The mechanical properties of the AlNbTiV alloy are rather unexpected for solid solution alloy—it has poor ductility at room

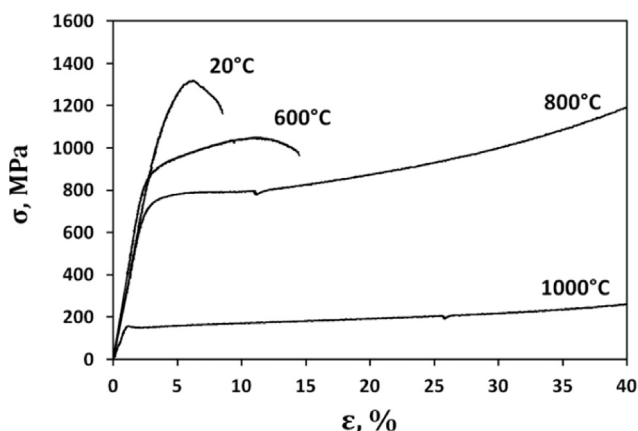


Fig. 2. Stress–strain compression curves of the AlNbTiV alloy at given temperatures.

Table 1

Compression mechanical properties of the AlNbTiV alloy.

T (°C)	$\sigma_{0.2}$ (MPa)	σ_p (MPa)	ϵ (%)
20	1020	1318	5
600	810	1050	12
800	685	–	–
1000	158	–	–

temperature but maintain reasonably high compressive strength at temperatures below 1000 °C. The comparison of specific yield strengths of the AlNbTiV HEA and previously reported CrNbTiVZr, CrNbTiZr [6], $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$ and $\text{Al}_{0.5}\text{NbTa}_{0.8}\text{Ti}_{1.5}\text{V}_{0.2}\text{Zr}$ [7] alloys is even more surprising (Fig. 3). The compared HEAs had multiphase structure beneficial for high temperature strength: the CrNbTiVZr and CrNbTiZr alloys contained bcc and Laves phases [5] whereas the $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$ and $\text{Al}_{0.5}\text{NbTa}_{0.8}\text{Ti}_{1.5}\text{V}_{0.2}\text{Zr}$ alloys were composed from two bcc phases [7]. The AlNbTiV alloy has the lowest specific yield strength among the alloys at room temperature and at 600 °C. But at temperature of 800 °C the AlNbTiV alloy is outperformed only by the $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$ alloy, whereas other alloys have considerably lower specific strength. Finally, at 1000 °C the specific strength of the AlNbTiV alloy is nearly the same as of CrNbTiVZr, CrNbTiZr and $\text{Al}_{0.5}\text{NbTa}_{0.8}\text{Ti}_{1.5}\text{V}_{0.2}\text{Zr}$ alloys but is about 3 times lower than strength of the $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$.

Unusual mechanical properties of AlNbTiV alloy can be attributed to large Al content. Effect of Al on mechanical properties of single bcc phase refractory HEAs was studied on $\text{Al}_{0.4}\text{Hf}_{0.6}\text{NbTaTiZr}$ and

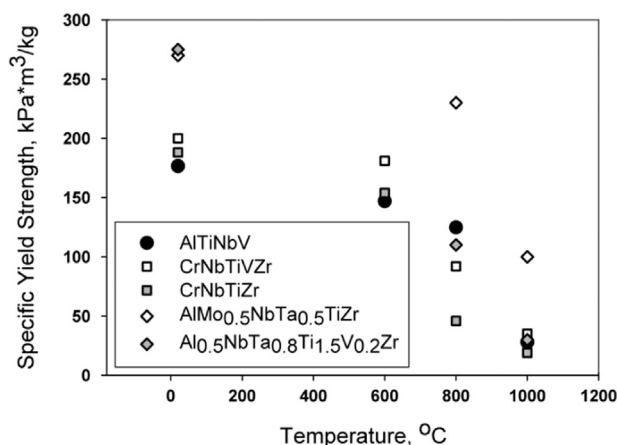


Fig. 3. Comparison between specific yield strength of the AlNbTiV alloy and CrNbTiVZr, CrNbTiZr [6], AlMo_{0.5}NbTa_{0.5}TiZr and Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr [7] alloys.

HfNbTaTiZr alloys with nearly identical microstructure [8]. The room temperature strength of the Al-containing alloy was almost two times higher than of HfNbTaTiZr, however, at cost of decreased ductility. It was proposed that atoms of Al form the strong chemical bonds with atoms of other constitutive elements [8], which is mirrored in highly negative enthalpy of mixing between corresponding atomic pairs [16]. But at temperature of 1000 °C the Al_{0.4}Hf_{0.6}NbTaTiZr and HfNbTaTiZr alloys had almost the same strength, most probably due to weakening of the chemical bonds, which is consistent with rapid decrease of strength of the AlNbTiV alloy at 1000 °C. Therefore, Al is likely to be responsible for high compressive strength of the AlNbTiV alloy. On the other hand, Al should be the reason of poor ductility of the AlNbTiV alloy at ambient temperature. Thus one can conclude that by tailoring the Al content in the Al–Nb–Ti–V system it is possible to control the mechanical properties of the alloys; increase of Al content will result in strengthening and loss of ductility.

4. Conclusions

In this work, the structure, density and mechanical properties of novel AlNbTiV high entropy alloy were examined. The alloy had single bcc phase coarse-grained structure and low density of 5.59 g cm^{−3} after homogenization. The compressive yield strength of the alloy gradually decreased from 1020 MPa at room temperature to 685 MPa

at 800 °C, and then dropped to 158 MPa at 1000 °C. The comparison between specific strengths of the AlNbTiV alloy and previously reported multiphase refractory HEAs has demonstrated no significant difference. High compressive strength was attributed to effect of Al. Potential ways to optimize composition of the alloy are proposed.

Acknowledgements

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